Tata Institute of Fundamental Research
Survey No. 36/P, Gopanpally Village, Serilingampally, Ranga Reddy Dist., Hyderabad – 500 046

Internal Webinar

Application of atomistic simulations towards mechanistic elucidation of therapeutically relevant proteins

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Understanding the dynamics AMA1-RON2 interaction is a therapeutically important research problem and role of specific domains is furthermore crucial because of the immense therapeutic potential this partnership offers. I have applied atomistic molecular dynamics coupled with biophysical experiments to quantitatively enumerate specific roles of different residues involved in the process. Subsequently I have tried to understand the molecular mechanism of binding for different chemically modified RON2 like ligands inspired from closing of domain II loop and its potential influence on the overall system. In a separate but related work, I have re-designed few peptide inhibitors against RON2 initially obtained from phage display through one of our collaborators. Additionally, I have described some preliminary results of initial virtual screening that aimed to rapidly discover lead D-peptides for further evaluation, by molecular docking against main protease (M^{pro}) of SARS-CoV-2. The final problem is regarding one of the most functionally active lectins, galectin-3 is distinctively known for its specific binding affinity towards beta-galactoside and is an important cancer target. Although available crystal structures are able to show the end-state bound poses, it is far from known the exact binding mechanism and possibility of formation of intermediate states. I have used molecular dynamics to elucidate the dynamical binding process of N-acetyllactosamine and one of its synthetic derivatives with human galectin-3.

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11:30 AM